

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 9.91e-09 mmHg

Global applicability domain: Inside

Local applicability domain index: 3.33e-01

Confidence level: 4.28e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>1,2,3,4,6-Pentachloronaphthalene</div> <div>Measured: 8.70e-09</div> <div>Predicted: 1.71e-06</div>	<div>Image not found</div> <div>Hexazinone</div> <div>Measured: 1.50e-09</div> <div>Predicted: 4.91e-07</div>	<div>Image not found</div> <div>2,3',4-Trichlorodiphenyl ether</div> <div>Measured: 1.20e-09</div> <div>Predicted: 1.55e-04</div>
<div>Image not found</div> <div>Furilazole</div> <div>Measured: 4.80e-09</div> <div>Predicted: 2.80e-04</div>	<div>Image not found</div> <div>Thenylchlor</div> <div>Measured: 2.41e-06</div> <div>Predicted: 6.04e-07</div>	